

Product Name: SR 3576

Catalog No.: 5044

Batch No.: 1

CAS Number: 1164153-22-3

IUPAC Name: 3-[4-[[[(3-Methylphenyl)amino]carbonyl]amino]-1H-pyrazol-1-yl]-N-(3,4,5-trimethoxyphenyl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₂₇N₅O₅·¼H₂O

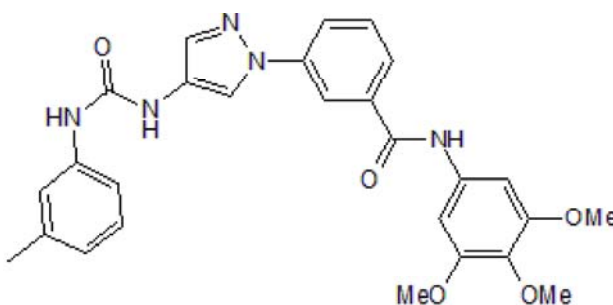
Batch Molecular Weight: 506.03

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.65 (Ethyl acetate:Methanol [9:1])

HPLC: Shows 97.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.08	5.48	13.84
Found	63.94	5.44	13.68

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Description:

Highly potent and selective JNK3 inhibitor ($IC_{50} = 7$ nM); exhibits > 2800-fold selectivity over p38.

Physical and Chemical Properties:

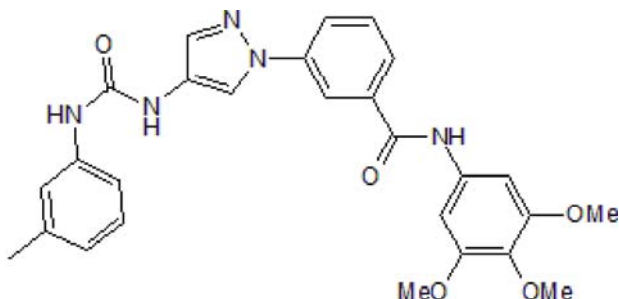
Batch Molecular Formula: $C_{27}H_{27}N_5O_5 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 506.03

Physical Appearance: Off White solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Kamenecka et al (2009) Structure-activity relationships and X-ray structures describing the selectivity of aminopyrazole inhibitors for c-Jun N-terminal kinase 3 (JNK3) over p38. *J Biol Chem.* **284** 12853. PMID: 19261605.

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